Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:10 PM EDT

PDB ID	:	3U8A
Title	:	Crystal structure of monomeric reversibly photoswitchable red fluorescent protein rsTagRFP in the OFF state
Authors	:	Pletnev, S.
Deposited on	:	2011-10-16
Resolution	:	1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

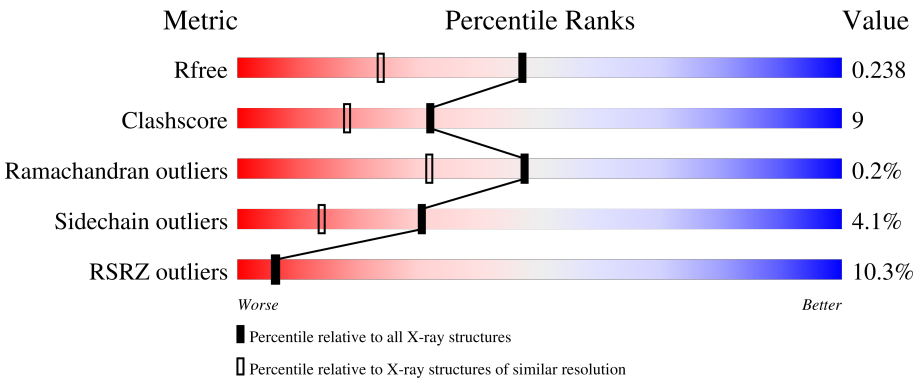
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	8%, 73%, 18%, •, 8%
1	B	243	10%, 75%, 16%, •, 8%
1	C	243	8%, 74%, 14%, 5%, 8%
1	D	243	12%, 77%, 14%, •, 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7676 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fluorescent protein rsTagRFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1786	1135	304	334	13	0	0	0
1	B	224	1786	1135	304	334	13	0	0	0
1	C	224	1786	1135	304	334	13	0	0	0
1	D	224	1786	1135	304	334	13	0	0	0

- Molecule 2 is water.

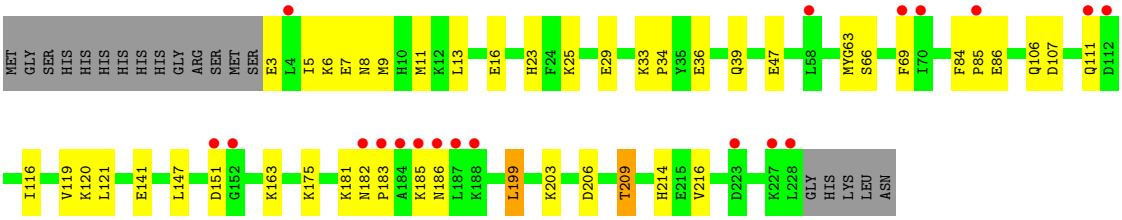
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	142	142	142	0	0
2	B	128	128	128	0	0
2	C	146	146	146	0	0
2	D	116	116	116	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

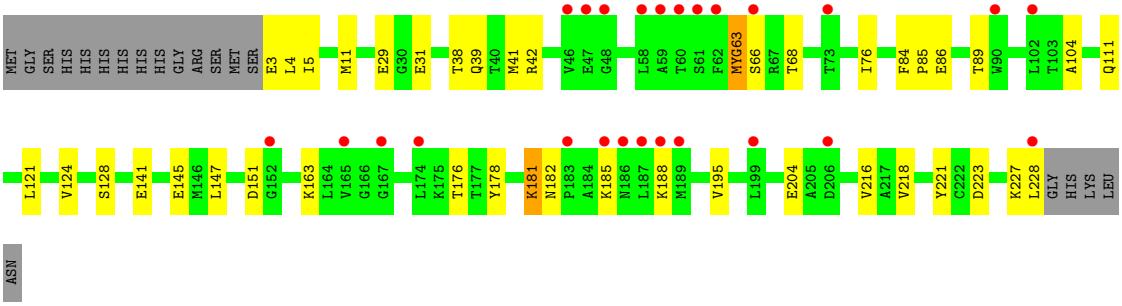
• Molecule 1: Fluorescent protein rsTagRFP

Chain A:



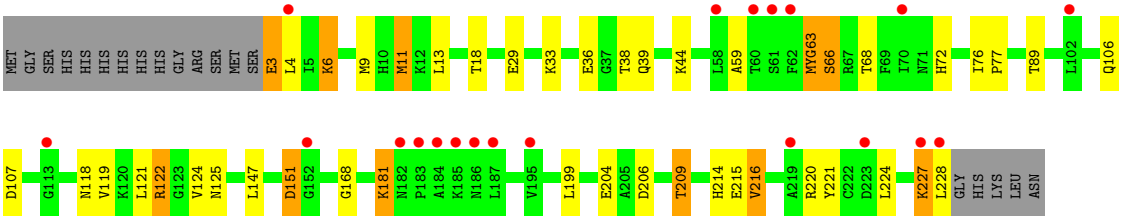
• Molecule 1: Fluorescent protein rsTagRFP

Chain B:



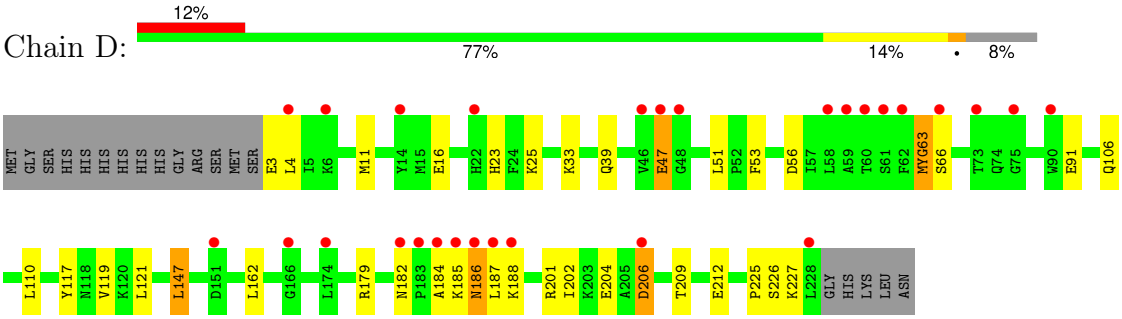
• Molecule 1: Fluorescent protein rsTagRFP

Chain C:



• Molecule 1: Fluorescent protein rsTagRFP

Chain D:


12%
77%
14%
8%
MET GLY SER HIS HIS HIS HIS HIS HIS GLY ARG SER MET SER E3 L4 I5 K6 M11 Y14 M15 E16 H22 H23 F24 K25 K33 Q39 V46 E47 G48 L51 P52 F53 D56 I57 L58 A59 T60 S61 F62 MYG63 S66 T73 Q74 G75 W90 E91 Q106
L110 Y117 N118 V119 K120 L121 L147 D151 L162 G166 L174 R179 N182 P183 A184 K185 N186 L187 K188 R201 I202 K203 E204 A205 D206 T209 E212 P225 S226 K227 L228 GLY HIS LYS LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.75Å 69.64Å 73.95Å 78.61° 83.77° 72.16°	Depositor
Resolution (Å)	26.65 – 1.78 29.56 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.9 (26.65-1.78) 93.9 (29.56-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.182 , 0.235 0.183 , 0.238	Depositor DCC
R_{free} test set	1650 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7676	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.83	0/1804	0.81	2/2435 (0.1%)
1	B	0.77	3/1804 (0.2%)	0.74	0/2435
1	C	0.84	1/1804 (0.1%)	0.81	2/2435 (0.1%)
1	D	0.73	0/1804	0.77	1/2435 (0.0%)
All	All	0.79	4/7216 (0.1%)	0.78	5/9740 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	VAL	CB-CG1	-6.57	1.39	1.52
1	B	104	ALA	CA-CB	-5.33	1.41	1.52
1	B	145	GLU	CG-CD	5.19	1.59	1.51
1	C	66	SER	N-CA	-5.01	1.36	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	LEU	CA-CB-CG	-6.76	99.75	115.30
1	A	199	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	147	LEU	CA-CB-CG	-5.48	102.69	115.30
1	C	72	HIS	CB-CA-C	5.28	120.95	110.40
1	A	147	LEU	CA-CB-CG	-5.13	103.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1786	0	1744	35	0
1	B	1786	0	1744	30	0
1	C	1786	0	1743	37	0
1	D	1786	0	1744	27	0
2	A	142	0	0	5	0
2	B	128	0	0	5	0
2	C	146	0	0	7	0
2	D	116	0	0	2	0
All	All	7676	0	6975	125	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HE2	2:A:317:HOH:O	1.69	0.93
1:B:185:LYS:HD3	2:B:256:HOH:O	1.69	0.91
1:C:6:LYS:HA	1:C:6:LYS:HE2	1.56	0.88
1:C:68:THR:HG23	2:C:256:HOH:O	1.75	0.87
1:B:3:GLU:HA	2:B:389:HOH:O	1.76	0.85
1:A:206:ASP:HB2	1:A:209:THR:HG22	1.59	0.81
1:D:182:ASN:ND2	1:D:185:LYS:HB2	1.97	0.80
1:C:151:ASP:OD2	1:C:151:ASP:O	2.01	0.77
1:D:39:GLN:HE22	1:D:66:SER:HB3	1.50	0.76
1:A:119:VAL:O	1:A:120:LYS:HD3	1.88	0.74
1:B:121:LEU:C	1:B:121:LEU:HD12	2.10	0.72
1:A:111:GLN:HG2	1:A:116:ILE:HG13	1.71	0.71
1:A:119:VAL:C	1:A:120:LYS:HD3	2.12	0.70
1:A:5:ILE:HA	1:A:9:MET:CE	2.23	0.69
1:D:182:ASN:CG	1:D:185:LYS:HB2	2.12	0.69
1:C:9:MET:HG2	2:C:310:HOH:O	1.93	0.69
1:A:5:ILE:HA	1:A:9:MET:HE2	1.76	0.68
1:A:39:GLN:HE22	1:A:66:SER:HB3	1.59	0.68
1:A:214:HIS:HD2	2:A:311:HOH:O	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:OD1	2:C:367:HOH:O	2.12	0.66
1:D:206:ASP:HB2	1:D:209:THR:OG1	1.95	0.66
1:C:121:LEU:C	1:C:121:LEU:HD12	2.16	0.66
1:C:106:GLN:HG3	1:C:119:VAL:HG22	1.79	0.65
1:C:227:LYS:N	1:C:227:LYS:HD2	2.11	0.64
1:D:25:LYS:HB2	1:D:47:GLU:HG3	1.78	0.64
1:B:41:MET:HB2	1:B:63:NRQ:CE	2.27	0.63
1:A:6:LYS:H	1:A:9:MET:CE	2.12	0.63
1:D:202:ILE:HB	1:D:212:GLU:HG2	1.80	0.63
1:D:4:LEU:HD22	1:D:110:LEU:HD23	1.79	0.63
1:C:18:THR:HG21	1:C:122:ARG:NH1	2.15	0.62
1:A:182:ASN:HD22	1:A:185:LYS:HD2	1.66	0.61
1:C:204:GLU:HG3	2:C:526:HOH:O	2.00	0.61
1:C:89:THR:HG23	1:C:181:LYS:HD2	1.83	0.60
1:D:66:SER:HG	1:D:117:TYR:HH	1.49	0.60
1:A:106:GLN:NE2	2:A:316:HOH:O	2.35	0.60
1:C:6:LYS:HA	1:C:6:LYS:CE	2.31	0.59
1:D:121:LEU:HD12	1:D:121:LEU:C	2.23	0.59
1:C:39:GLN:HE22	1:C:66:SER:CB	2.16	0.58
1:C:33:LYS:HD2	1:C:36:GLU:OE1	2.03	0.58
2:B:302:HOH:O	1:C:168:GLY:HA2	2.04	0.56
1:B:76:ILE:HG12	1:B:221:TYR:CZ	2.40	0.56
1:A:175:LYS:HE3	2:A:442:HOH:O	2.06	0.56
1:A:120:LYS:HD3	1:A:120:LYS:N	2.21	0.55
1:C:76:ILE:HG12	1:C:221:TYR:CZ	2.40	0.55
1:D:182:ASN:HD22	1:D:185:LYS:HD2	1.71	0.55
1:A:66:SER:N	2:A:300:HOH:O	2.39	0.54
1:A:111:GLN:HG2	1:A:116:ILE:CG1	2.36	0.54
1:A:107:ASP:OD1	1:A:181:LYS:HE2	2.07	0.54
1:C:77:PRO:HA	2:C:239:HOH:O	2.08	0.54
1:A:214:HIS:CG	1:D:227:LYS:HE2	2.44	0.53
1:A:86:GLU:HG2	1:A:182:ASN:HB2	1.90	0.53
1:D:51:LEU:HD13	1:D:53:PHE:CZ	2.44	0.53
1:A:121:LEU:C	1:A:121:LEU:HD12	2.29	0.53
1:B:11:MET:HE3	1:B:31:GLU:HA	1.91	0.52
1:C:220:ARG:HG3	1:C:221:TYR:O	2.10	0.52
1:A:33:LYS:HB2	1:A:36:GLU:HB2	1.91	0.52
1:A:6:LYS:O	1:A:8:ASN:N	2.42	0.52
1:C:59:ALA:HB1	1:C:199:LEU:HD21	1.92	0.51
1:C:63:NRQ:HB12	1:C:215:GLU:OE1	2.10	0.51
1:A:16:GLU:OE2	1:A:23:HIS:NE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:NRQ:O2	1:C:63:NRQ:HD2	2.11	0.51
1:A:86:GLU:H	1:A:86:GLU:CD	2.13	0.51
1:B:111:GLN:NE2	2:B:396:HOH:O	2.38	0.51
1:A:33:LYS:HD2	1:A:36:GLU:HG3	1.92	0.51
1:B:41:MET:HB2	1:B:63:NRQ:HE3	1.92	0.51
1:B:68:THR:HG23	2:B:245:HOH:O	2.11	0.50
1:D:39:GLN:NE2	1:D:66:SER:HB3	2.24	0.50
1:B:41:MET:CB	1:B:63:NRQ:CE	2.88	0.50
1:B:141:GLU:CD	1:B:163:LYS:HE2	2.32	0.50
1:D:106:GLN:HG3	1:D:119:VAL:HG22	1.93	0.50
1:B:147:LEU:HD12	1:B:195:VAL:HG23	1.94	0.49
1:B:86:GLU:HG2	1:B:182:ASN:HB2	1.94	0.49
1:C:11:MET:HE1	1:C:39:GLN:HB2	1.94	0.49
1:B:41:MET:CB	1:B:63:NRQ:HE3	2.42	0.49
1:D:186:ASN:HD22	1:D:187:LEU:N	2.10	0.49
1:C:38:THR:HG22	1:C:216:VAL:HG13	1.94	0.48
1:B:89:THR:HG23	1:B:181:LYS:HD2	1.94	0.48
1:A:6:LYS:H	1:A:9:MET:HE1	1.79	0.47
1:C:18:THR:CG2	1:C:122:ARG:NH1	2.77	0.47
1:B:121:LEU:HD12	1:B:121:LEU:O	2.14	0.47
1:B:218:VAL:HG23	1:C:224:LEU:HD21	1.96	0.47
1:C:206:ASP:O	1:C:209:THR:HB	2.14	0.47
1:B:84:PHE:HB3	1:B:85:PRO:HA	1.97	0.47
1:B:3:GLU:HG3	1:B:5:ILE:H	1.80	0.47
1:A:141:GLU:OE2	1:A:163:LYS:HD3	2.15	0.46
1:C:63:NRQ:O3	1:C:106:GLN:NE2	2.40	0.46
1:A:13:LEU:C	1:A:13:LEU:HD23	2.35	0.46
1:C:44:LYS:HE2	2:C:333:HOH:O	2.14	0.46
1:D:184:ALA:HB3	2:D:525:HOH:O	2.16	0.46
1:D:206:ASP:N	1:D:206:ASP:OD1	2.48	0.46
1:A:25:LYS:HD2	1:A:47:GLU:OE1	2.15	0.46
1:C:11:MET:CE	1:C:39:GLN:HB2	2.46	0.46
1:C:151:ASP:O	1:C:151:ASP:CG	2.53	0.46
1:B:63:NRQ:HD2	1:B:63:NRQ:O2	2.16	0.46
1:A:206:ASP:O	1:A:209:THR:HB	2.16	0.45
1:C:124:VAL:O	1:C:125:ASN:HB2	2.16	0.45
1:B:147:LEU:CD1	1:B:195:VAL:HG23	2.46	0.45
1:C:121:LEU:HD12	1:C:121:LEU:O	2.17	0.45
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.82	0.44
1:B:4:LEU:CD1	1:B:85:PRO:HB3	2.48	0.44
1:C:3:GLU:HG2	1:C:4:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLU:CD	1:D:179:ARG:HH12	2.21	0.44
1:D:182:ASN:ND2	1:D:185:LYS:HD2	2.32	0.44
1:A:84:PHE:HB3	1:A:85:PRO:HA	1.99	0.44
1:D:201:ARG:HD2	1:D:204:GLU:OE1	2.17	0.43
1:D:16:GLU:OE2	1:D:23:HIS:NE2	2.46	0.43
1:B:38:THR:HG22	1:B:216:VAL:HG13	2.01	0.43
1:C:107:ASP:OD1	1:C:181:LYS:HE3	2.19	0.43
1:B:29:GLU:OE2	1:B:42:ARG:NH2	2.52	0.43
1:A:6:LYS:H	1:A:9:MET:HE2	1.82	0.43
1:B:4:LEU:HD11	1:B:85:PRO:HB3	2.01	0.43
1:B:228:LEU:HD12	2:C:370:HOH:O	2.17	0.43
1:D:56:ASP:HB3	1:D:162:LEU:HD11	2.00	0.42
1:B:227:LYS:HD3	1:C:214:HIS:CG	2.55	0.42
1:A:216:VAL:HG11	1:D:225:PRO:HD2	2.01	0.42
1:C:13:LEU:C	1:C:13:LEU:HD23	2.40	0.42
1:D:63:NRQ:HD2	1:D:63:NRQ:O2	2.20	0.42
1:D:33:LYS:HB3	2:D:277:HOH:O	2.19	0.42
1:D:188:LYS:HA	1:D:188:LYS:HD3	1.83	0.42
1:B:176:THR:HG21	1:B:178:TYR:CZ	2.55	0.41
1:A:34:PRO:HA	1:A:69:PHE:HA	2.02	0.41
1:B:141:GLU:OE1	1:B:163:LYS:HE2	2.21	0.41
1:A:181:LYS:O	1:A:183:PRO:HD3	2.21	0.41
1:C:121:LEU:C	1:C:121:LEU:CD1	2.87	0.41
1:D:206:ASP:HB2	1:D:209:THR:HG1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/243 (90%)	209 (95%)	9 (4%)	1 (0%)	29 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	219/243 (90%)	215 (98%)	3 (1%)	1 (0%)	29	14
1	C	219/243 (90%)	214 (98%)	5 (2%)	0	100	100
1	D	219/243 (90%)	211 (96%)	8 (4%)	0	100	100
All	All	876/972 (90%)	849 (97%)	25 (3%)	2 (0%)	47	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	B	151	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/206 (92%)	182 (96%)	8 (4%)	30	13
1	B	190/206 (92%)	185 (97%)	5 (3%)	46	29
1	C	190/206 (92%)	179 (94%)	11 (6%)	20	6
1	D	190/206 (92%)	183 (96%)	7 (4%)	34	17
All	All	760/824 (92%)	729 (96%)	31 (4%)	30	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	11	MET
1	A	29	GLU
1	A	151	ASP
1	A	186	ASN
1	A	199	LEU
1	A	203	LYS
1	A	209	THR
1	B	128	SER

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Mol	Chain	Res	Type
1	B	181	LYS
1	B	188	LYS
1	B	204	GLU
1	B	223	ASP
1	C	3	GLU
1	C	6	LYS
1	C	11	MET
1	C	29	GLU
1	C	122	ARG
1	C	151	ASP
1	C	181	LYS
1	C	209	THR
1	C	216	VAL
1	C	227	LYS
1	C	228	LEU
1	D	3	GLU
1	D	11	MET
1	D	47	GLU
1	D	147	LEU
1	D	186	ASN
1	D	206	ASP
1	D	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	213	GLN
1	B	8	ASN
1	B	10	HIS
1	C	23	HIS
1	C	39	GLN
1	D	8	ASN
1	D	10	HIS
1	D	82	GLN
1	D	186	ASN
1	D	213	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NRQ	B	63	1	24,24,25	1.80	5 (20%)	24,32,34	3.38	9 (37%)
1	NRQ	A	63	1	24,24,25	1.75	5 (20%)	24,32,34	3.08	10 (41%)
1	NRQ	D	63	1	24,24,25	1.60	4 (16%)	24,32,34	2.68	8 (33%)
1	NRQ	C	63	1	24,24,25	1.68	4 (16%)	24,32,34	2.72	9 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	B	63	1	-	5/9/31/32	0/2/2/2
1	NRQ	A	63	1	-	5/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	5/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	5/9/31/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	NRQ	CA1-N1	5.59	1.40	1.27
1	B	63	NRQ	CA1-N1	4.93	1.38	1.27
1	C	63	NRQ	CA1-N1	4.89	1.38	1.27
1	A	63	NRQ	CG2-CB2	-4.84	1.38	1.46
1	B	63	NRQ	C1-CA1	3.79	1.53	1.48
1	A	63	NRQ	CA1-N1	3.79	1.36	1.27
1	C	63	NRQ	CA2-C2	3.78	1.52	1.48
1	B	63	NRQ	CB2-CA2	3.19	1.38	1.35
1	A	63	NRQ	CA2-C2	3.03	1.51	1.48
1	D	63	NRQ	CG2-CB2	-3.00	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	NRQ	CG2-CB2	-2.86	1.41	1.46
1	A	63	NRQ	CD1-CG2	2.67	1.44	1.39
1	C	63	NRQ	CG2-CB2	-2.53	1.42	1.46
1	B	63	NRQ	CA2-C2	2.30	1.51	1.48
1	D	63	NRQ	CB2-CA2	2.06	1.37	1.35
1	D	63	NRQ	O2-C2	-2.04	1.18	1.23
1	A	63	NRQ	CB2-CA2	2.03	1.37	1.35
1	C	63	NRQ	CD1-CG2	2.03	1.43	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	NRQ	O2-C2-CA2	10.12	137.48	131.02
1	A	63	NRQ	CB2-CA2-C2	7.83	131.85	122.36
1	D	63	NRQ	CG2-CB2-CA2	7.22	138.45	129.87
1	C	63	NRQ	CB2-CA2-C2	7.15	131.02	122.36
1	A	63	NRQ	CG2-CB2-CA2	6.81	137.96	129.87
1	B	63	NRQ	CB2-CA2-C2	6.77	130.56	122.36
1	D	63	NRQ	CB2-CA2-C2	6.63	130.39	122.36
1	B	63	NRQ	CG2-CB2-CA2	6.56	137.66	129.87
1	C	63	NRQ	CG2-CB2-CA2	5.89	136.87	129.87
1	A	63	NRQ	CB2-CA2-N2	-4.97	122.01	128.76
1	A	63	NRQ	C3-CA3-N3	4.94	123.66	112.43
1	C	63	NRQ	CB2-CA2-N2	-4.50	122.65	128.76
1	B	63	NRQ	CB2-CA2-N2	-4.15	123.12	128.76
1	C	63	NRQ	O2-C2-CA2	4.14	133.66	131.02
1	B	63	NRQ	C3-CA3-N3	4.13	121.82	112.43
1	D	63	NRQ	CB2-CA2-N2	-4.04	123.27	128.76
1	A	63	NRQ	O2-C2-CA2	4.03	133.59	131.02
1	C	63	NRQ	C3-CA3-N3	4.01	121.55	112.43
1	A	63	NRQ	C2-CA2-N2	-4.00	106.08	108.95
1	D	63	NRQ	C2-CA2-N2	-3.77	106.25	108.95
1	B	63	NRQ	C2-CA2-N2	-3.74	106.27	108.95
1	C	63	NRQ	C2-CA2-N2	-3.70	106.30	108.95
1	D	63	NRQ	O2-C2-CA2	3.56	133.30	131.02
1	D	63	NRQ	C3-CA3-N3	3.40	120.17	112.43
1	B	63	NRQ	O2-C2-N3	-3.35	117.33	124.31
1	C	63	NRQ	CA2-C2-N3	2.50	105.60	103.50
1	A	63	NRQ	CD1-CG2-CD2	-2.50	113.94	117.65
1	D	63	NRQ	CA2-N2-C1	2.50	108.69	104.09
1	A	63	NRQ	CA3-N3-C1	2.37	133.07	128.39
1	A	63	NRQ	CA2-C2-N3	2.37	105.49	103.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	NRQ	CA3-N3-C1	2.37	133.06	128.39
1	A	63	NRQ	CA2-N2-C1	2.34	108.40	104.09
1	D	63	NRQ	CA2-C2-N3	2.20	105.35	103.50
1	C	63	NRQ	CA3-N3-C1	2.12	132.57	128.39
1	B	63	NRQ	CA2-N2-C1	2.12	107.99	104.09
1	C	63	NRQ	N3-C1-N2	2.02	115.02	112.62

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	NRQ	CA1-CB1-CG1-SD
1	A	63	NRQ	C2-CA2-CB2-CG2
1	A	63	NRQ	C3-CA3-N3-C1
1	A	63	NRQ	C3-CA3-N3-C2
1	B	63	NRQ	C1-CA1-CB1-CG1
1	B	63	NRQ	C2-CA2-CB2-CG2
1	B	63	NRQ	C3-CA3-N3-C1
1	C	63	NRQ	C2-CA2-CB2-CG2
1	C	63	NRQ	C3-CA3-N3-C1
1	C	63	NRQ	C3-CA3-N3-C2
1	D	63	NRQ	C1-CA1-CB1-CG1
1	D	63	NRQ	C2-CA2-CB2-CG2
1	D	63	NRQ	C3-CA3-N3-C1
1	B	63	NRQ	N2-CA2-CB2-CG2
1	B	63	NRQ	C3-CA3-N3-C2
1	D	63	NRQ	C3-CA3-N3-C2
1	A	63	NRQ	N2-CA2-CB2-CG2
1	C	63	NRQ	N2-CA2-CB2-CG2
1	D	63	NRQ	N2-CA2-CB2-CG2
1	C	63	NRQ	CA1-CB1-CG1-SD

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRQ	5	0
1	D	63	NRQ	1	0
1	C	63	NRQ	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	223/243 (91%)	0.44	19 (8%)	10	10	26, 46, 83, 138	0
1	B	223/243 (91%)	0.59	25 (11%)	5	5	25, 49, 79, 102	0
1	C	223/243 (91%)	0.43	20 (8%)	9	9	26, 47, 78, 123	0
1	D	223/243 (91%)	0.68	28 (12%)	3	3	28, 51, 80, 146	0
All	All	892/972 (91%)	0.53	92 (10%)	6	6	25, 48, 81, 146	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	ALA	10.3
1	D	187	LEU	7.5
1	D	184	ALA	7.1
1	B	187	LEU	6.4
1	D	183	PRO	6.3
1	D	186	ASN	6.1
1	C	228	LEU	6.0
1	A	228	LEU	5.7
1	C	152	GLY	5.4
1	A	183	PRO	5.1
1	B	188	LYS	4.8
1	A	187	LEU	4.7
1	B	228	LEU	4.7
1	D	185	LYS	4.5
1	C	183	PRO	4.5
1	A	186	ASN	4.4
1	C	186	ASN	4.4
1	B	189	MET	4.4
1	B	62	PHE	4.0
1	B	185	LYS	4.0
1	A	185	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	60	THR	3.9
1	D	182	ASN	3.9
1	B	90	TRP	3.7
1	B	66	SER	3.7
1	D	90	TRP	3.6
1	D	59	ALA	3.6
1	A	4	LEU	3.6
1	A	70	ILE	3.6
1	B	152	GLY	3.6
1	C	4	LEU	3.5
1	B	60	THR	3.5
1	B	165	VAL	3.5
1	B	48	GLY	3.4
1	D	4	LEU	3.3
1	D	206	ASP	3.3
1	B	46	VAL	3.3
1	D	151	ASP	3.3
1	D	62	PHE	3.3
1	B	59	ALA	3.3
1	A	152	GLY	3.3
1	C	185	LYS	3.3
1	D	228	LEU	3.2
1	C	70	ILE	3.2
1	D	58	LEU	3.1
1	B	174	LEU	3.0
1	D	61	SER	3.0
1	B	183	PRO	2.9
1	D	73	THR	2.8
1	C	62	PHE	2.8
1	C	184	ALA	2.8
1	B	199	LEU	2.8
1	A	182	ASN	2.8
1	A	58	LEU	2.7
1	C	58	LEU	2.7
1	D	48	GLY	2.7
1	B	47	GLU	2.6
1	B	73	THR	2.6
1	D	75	GLY	2.5
1	D	166	GLY	2.5
1	C	219	ALA	2.5
1	C	61	SER	2.4
1	C	195	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	2.4
1	B	102	LEU	2.4
1	B	61	SER	2.4
1	A	188	LYS	2.4
1	D	188	LYS	2.4
1	A	111	GLN	2.4
1	D	14	TYR	2.3
1	C	182	ASN	2.3
1	A	227	LYS	2.3
1	B	167	GLY	2.3
1	D	174	LEU	2.3
1	C	113	GLY	2.3
1	A	69	PHE	2.3
1	B	186	ASN	2.3
1	B	206	ASP	2.2
1	C	227	LYS	2.2
1	D	66	SER	2.2
1	A	223	ASP	2.1
1	C	187	LEU	2.1
1	C	223	ASP	2.1
1	A	112	ASP	2.1
1	A	151	ASP	2.1
1	D	47	GLU	2.1
1	D	46	VAL	2.0
1	D	6	LYS	2.0
1	D	22	HIS	2.0
1	C	102	LEU	2.0
1	C	60	THR	2.0
1	A	85	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	NRQ	A	63	23/24	0.86	0.19	36,44,58,102	0
1	NRQ	B	63	23/24	0.88	0.28	40,50,61,66	0
1	NRQ	C	63	23/24	0.90	0.15	41,50,58,59	0
1	NRQ	D	63	23/24	0.91	0.26	45,52,70,79	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.